MICROWAVE ANALOGUE FOR X-RAY DIFFRACTION PART II. SIZE OF THE SCATTERERS

G. S. SANYAL AND G. B. MITRA

INDIAN INSTITUTE OF TECHNOLOGY, KHARAGPUR

(*Received March* 8, 1961)

ABSTRACT. The variation with the azimuthal angle of scattering of amplitude of electromagnetic waves scattered by conducting spheres of sizes (a) comparable and (b) negligible with respect to the wave-length has been studied. A workable theoretical expression has been obtained and evaluated by carrying out numerical computations. The theoretical expressions to be computed contain high order Hankel functions, Legendre polynomials and their derivatives numerical values of which are not given in ordinarily available tables. These values have been calculated and used in the numerical computations. The resultant curves show that the conducting sphere with $2\pi a/\lambda = 2$, where 'a' is the radius of the sphere and λ the wavelength of the e.m. waves is the nearest approximation to several atoms as far as scattering behaviour towards X-rays is concerned.

I. INTRODUCTION

Recently, Allen (1955) and Mitra and Sanyal (1960) have studied the scattering of electromagnetic waves in the microwave region by three dimensional arrays of metallic scatterers. While Allen (1955) worked with metallic discs as scatterers, Mitra and Sanyal (1960) used small cylinders for the purpose. Such scatterers, however, can hardly be used to build a true analogue in the microwave region for the diffraction of X-rays by crystals. The scatterers which are meant to simulate the atoms in the crystal lattices lack the spherical or near spherical symmetry possessed by atoms. Moreover, the variation of amplitude of electromagnetic waves scattered by these scatterers with the azimuthal angle of scattering should be similar to the atomic scattering factor graphs to make the analogue serve any useful purpose. It appears obvious that a solid sphere of dielectric or conducting material and of a proper size should serve the purpose, more or less, adequately. Hence, it has been decided to investigate theoretically the scattering patterns of conducting spheres to find out the proper size whose scattering pattern will approximate to the atomic scattering factor graphs. Since ionic radii of atoms are of the order of X-ray wavelengths, it has been intuitively felt that the proper size of the diffracting sphere would probably be comparable to the wavelength used. The case of vanishing sphere-size has also been studied to investigate the effect of diminishing the sphere-size.

Although the problem of diffraction of electromagnetic waves by spheres and spheroids has been studied by various authors [Mie, (1908), Blumer (1925, 1926a, 1926b and 1926c)] investigations of the type envisaged by us have not been carried out so far. Hence it has been decided to plot the graphs of the amplitude of microwaves scattered by spheres against the azimuthal angle of scattering for conducting spheres of sizes given by $\rho = 6, \rho = 2$ and $\rho \rightarrow 0$ where $\rho = 2\pi a/\lambda$, 'a' being the radius of the sphere and λ the wavelength used. Only conducting spheres have been considered to render the already formidable numerical computations somewhat less complicated.

II. THEORETICAL CONSIDERATIONS

Let a plane electromagnetic wave, propagating in free-space along the z-axis and polarised linearly along the x-axis, be incident on a *perfectly conducting sphere* of radius 'a' located at the origin of a spherical co-ordinate system r, θ, ϕ as shown in Fig. 1. The scattering process will be such that the resultant electromagnetic field satisfies the boundary conditions on the surface of the sphere and also reduces to a plane wave at a large distance r. The expressions for the scattered electromagnetic fields have been given by Stratton (1941). Thus for an incident plane electromagnetic wave expressed as

$$\bar{E}_i = 1_x E_0 \exp i(\beta z - \omega t)$$

$$H_i = 1_y (E_0/\sqrt{\mu_0/\epsilon_0}) \exp i(\beta z - \omega t),$$

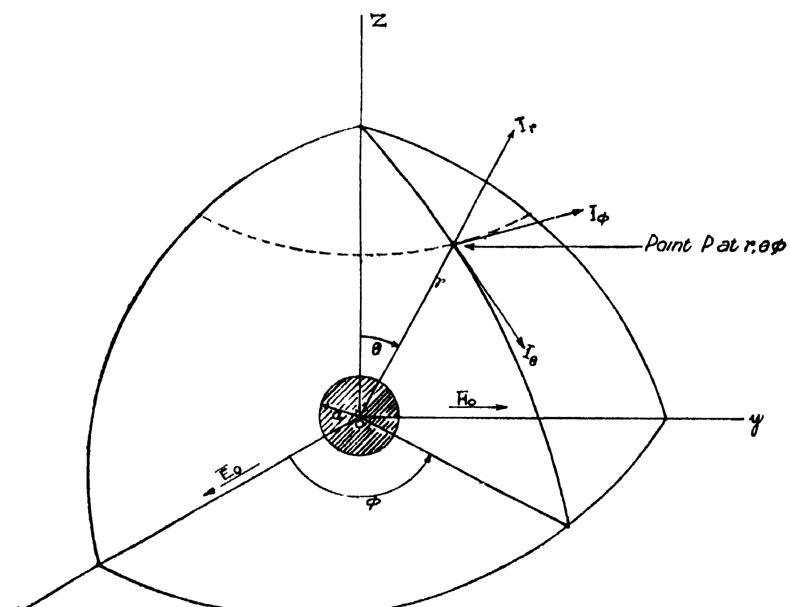

Fig. 1. Conducting sphere of radius 'a' located at the origin of a spherical coordinate system. 1_r, 1_θ, 1_ϕ are mutually orthogonal unit vectors at the point P.

the scattered electric field vector at any point $P(r, \theta, \phi)$ outside the sphere is

$$E_S = E_0 \exp(-i\omega t) \sum^{\infty} i^n \frac{2n+1}{n(n+1)} [a^S_n \bar{m}_{01n} - i\, b^S_n\, \bar{n}_{e1n}] \quad \ldots \quad (1)$$

where, E_0 is the amplitude of the incident electric field

β, the phase constant of the plane wave in free-space $= \omega\sqrt{\mu_0 \epsilon_0} = 2\pi/\lambda_0$, λ_0 being the free-space wavelength

μ_0, the permeability of free-space $= 1.257 \times 10^{-6}$ H/metre

ϵ_0, the permittivity of free-space $= 8.854 \times 10^{-12}$ F/metre

$\omega = 2\pi f$, f being the frequency of the incident wave

$\bar{m}_{01n}$, an odd vector function

$$= \bar{1}_\theta \left[\frac{1}{\sin\theta} h^{(1)}{}_n(\beta r) P^1{}_n (\cos\theta) \cos\phi \right]$$

$$- \bar{1}_\phi \left[h^{(1)}{}_n(\beta r) \frac{\partial P^1{}_n (\cos\theta)}{\partial\theta} \sin\phi \right]$$

$\bar{n}_{e1n}$ an even vector function

$$= \bar{1}_r \left[\frac{n(n+1)}{\beta r} h^{(1)}{}_n(\beta r) P^1{}_n (\cos\theta) \cos\phi \right]$$

$$+ \bar{1}_\theta \left[\frac{1}{\beta r} \frac{\partial\{\beta r h^{(1)}{}_n(\beta r)\}}{\partial(\beta r)} \frac{\partial P_n{}^1 (\cos\theta)}{\partial\theta} \cos\phi \right]$$

$$- \bar{1}_\phi \left[\frac{1}{\beta r \sin\theta} \frac{\partial\{\beta r h_n{}^{(1)}(\beta r)\}}{\partial(\beta r)} P^1{}_n (\cos\theta) \sin\phi \right]$$

$$a^S{}_n = -j_n(\rho)/h^{(1)}{}_n(\rho)$$

$$b^S{}_n = -\left[\frac{d}{d\rho} \{\rho j_m(\rho)\}\right] / \left[\frac{d}{d\rho} \{\rho h^{(1)}{}_n(\rho)\}\right]$$

$$j_n(\rho) = \sqrt{(\pi/2\rho)}\; J_{n+\frac{1}{2}}(\rho)$$

$$h^{(1)}{}_n(\rho) = \sqrt{(\pi/2\rho)}\; H^{(1)}{}_{n+\frac{1}{2}}(\rho)$$

$$\rho = 2\pi a/\lambda$$

$J_{n+\frac{1}{2}}$ and $H^{(1)}_{n+\frac{1}{2}}$ are respectively Bessel and first kind Hankel functions each of order $n+\frac{1}{2}$

$P^1_n(\cos\theta)$ is an associated Legendre polynomial.

The theoretical scattering pattern at a very large distance away from the conducting sphere may now be calculated from Eq.(1). The form given by Morse and Feshbach (1953) requires to be further simplified for direct computation and will not be used in this article. It is enough for our purpose to consider the variation of the electric field vector alone, since at a large distance the scattered field reduces to a uniform plane wave. The simplified asymptotic form of Eq. (1) valid at a large distance i.e. $\beta r >> 1$ and $r >> a$ may be arrived at by noting that

$$\mathrm{Lim.}_{\beta r>>1}\, h_n^{(1)}(\beta r) \to \frac{1}{\beta r}(-i)^{n+1}\exp(i\beta r)$$

$$\mathrm{Lim}_{\beta r>>1}\, \frac{1}{\beta r}\frac{d\{\beta r h_n^{(1)}(\beta r)\}}{d(\beta r)} \to \frac{1}{\beta r}(-i)^n \exp(i\beta r).$$

Substitution of the limiting values of the above two expressions in Eq.(1) yields the components of the scattered electric field vector at a large distance as

$$E_{Sr} = 0$$

$$E_{S\theta} = \frac{iE_0\cos\phi}{\beta r}\exp\, i(\beta r-\omega t)\,\times$$

$$\sum^{\infty}\frac{2n+1}{n(n+1)}\left[a_n{}^S\frac{P_n{}^1(\cos\theta)}{\sin\theta}+b_n{}^S\frac{dP_n{}^1(\cos\theta)}{d\theta}\right]$$

$$E_{S\phi} = \frac{iE_0\sin\phi}{\beta r}\exp\, i(\beta r-\omega t)\times$$

$$\sum^{\infty}\frac{2n+1}{n(n+1)}\left[a_n{}^S\frac{dP_n{}^1(\cos\theta)}{d\theta}+b_n{}^S\frac{P_n{}^1(\cos\theta)}{\sin\theta}\right] \qquad \ldots \quad (2)$$

The rate of convergence of the above expressions for the θ and ϕ components of the scattered field depends largely upon the convergence of $a_n{}^S$ and $b_n{}^S$ for successively increasing values of n. For values of ρ *large* compared to unity, both the terms inside the square brackets of Eq.(2) converge very slowly and the summation has to be carried out over a large value of n. In the special case when ρ is *finite* but very much less than unity, $a_n{}^S$ and $b_n{}^S$ can be expanded in powers of ρ giving to the first order of approximation

$$b_n{}^S \simeq -\frac{2}{3} i\rho^3 \qquad \text{for} \quad n=1$$

$$\simeq 0 \qquad \text{for} \quad n>1$$

$$a_n{}^S \simeq \frac{1}{3} i\rho^3 \qquad \text{for} \quad n=1$$

$$\simeq 0 \qquad \text{for} \quad n>1$$

Substitution of these values of $a_n{}^S$ and $b_n{}^S$ in Eq. (2) yields the scattered fields in the far zone due to a *finite but very small* conducting sphere as

$$E_{S\theta} = \frac{1}{2}\frac{E_0 \cos\phi}{\beta r}\rho^3(1-2\cos\theta)\exp i(\beta r-\omega t)$$

$$-\frac{2\pi^2 E_0 \cos\phi}{\lambda^2 r} a^3(1-2\cos\theta)\exp i(\beta r-\omega t)$$

$$E_{S\varphi} = \frac{1}{2}\frac{E_0 \sin\phi}{\beta r}\rho^3(2-\cos\theta)\exp i(\beta r-\omega t)$$

$$-\frac{2\pi^2 E_0 \sin\phi}{\lambda^2 r} a^3(2-\cos\theta)\exp i(\beta r-\omega t) \tag{3}$$

III. NUMERICAL COMPUTATION

To study the nature of the variation of the scattered field with the polar angle θ, the summation in Eq. (2) has to be performed over a sufficiently large value of n. In this article n has been so chosen that the numerical result may be correct to, at least, the third decimal place. Numerical computation for only $E_{S\varphi}$ and that too for three values of ρ, (i) $\rho \ll 1$ i.e., $a \ll \lambda$, (ii) $\rho = 2$ i.e., $a = \lambda/\pi$ and (iii) $\rho = 6$ i.e., $a \simeq \lambda$ has been carried out, since these results are singificant enough to indicate the general nature of variation of the scattered fields with θ and also to show the effect of the radius of the sphere on the scattering pattern. The first case e.g. $\rho \ll 1$ has been calculated using Eq. (3) and the other two cases by using Eq. (2).

Calculation of the coefficients $a_n{}^S$ and $b_n{}^S$ in Eq.(2) requires tables of j_n and $h_n{}^{(1)}$ functions and their derivatives. Since these tables are not available the coefficients were obtained as follows :

$$a_n{}^S = -\frac{j_n(\rho)}{h_n{}^{(1)}(\rho)} \qquad \frac{J_{n+\frac{1}{2}}(\rho)}{H_{n+\frac{1}{2}}{}^{(1)}(\rho)}$$

$$b_n{}^S = -\left[\frac{d}{d\rho}\{\rho j_n(\rho)\}\right] \Big/ \left[\frac{d}{d\rho}\{\rho\, h_n{}^{(1)}(\rho)\}\right]$$

$$= -\frac{J_{n+\frac{1}{2}}(\rho)+\rho[J_{(n-1)+\frac{1}{2}}(\rho)-J_{(n+1)+\frac{1}{2}}(\rho)]}{H_{n+\frac{1}{2}}{}^{(1)}(\rho)+\rho[H_{(n-1)+\frac{1}{2}}{}^{(1)}(\rho)-H_{(n+1)+\frac{1}{2}}{}^{(1)}(\rho)]}$$

The Hankel function $H_\nu{}^{(1)}$ itself was computed from the formula

$$H_\nu{}^{(1)}(x) = [J_{-\nu}(x) - J_\nu(x)\ \exp\ (-\nu\pi i)]/[i \sin \nu\pi]$$

and the tables for J_ν and $J_{-\nu}$ as given by Watson (1922).

Again the numerical computation of Eq.(2) requires the use of the tables of $P_n{}^1(\cos\theta)$ and its derivate for different values of n. Since these tables also are not available for large n, their values were computed and tabulated for the value of the order n up to 10 by using the recurrence relations :

$$P_{n+1}{}^1(\cos\theta) = [(2n+1)\cos\theta\ P_n{}^1(\cos\theta) - (n+1)P_{n-1}{}^1(\cos\theta)]/n$$

$$d/d\theta[P_n{}^1(\cos\theta)] = [nP_{n+1}{}^1(\cos\theta) - (n+1)\cos\theta\ P_n{}^1(\cos(\theta)]/\sin\theta$$

from the lower order polynomials given by Jahnke and Emde (1943).

Eq.(2) can now be evaluated term by term for successively increasing values of n and the summation obtained.

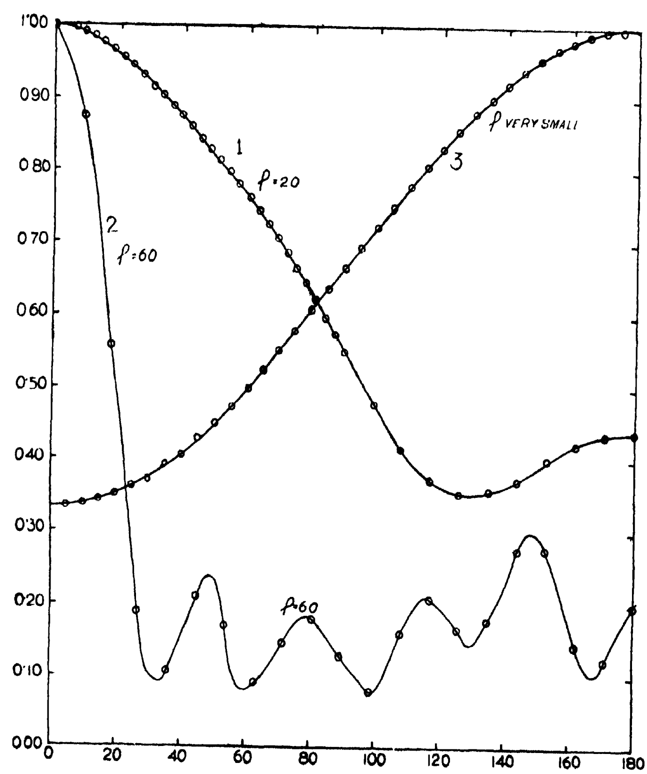

Fig. 2. Scattering patterns of conducting spheres of several sizes (Curve 1, $\rho = 2.0$, Curve 2, $\rho = 6.0$ and Curve 3, ρ very small).

IV. DISCUSSIONS

The theoretical scattering patterns for conducting spheres as computed for the three cases mentioned before are plotted graphically in Fig. 2. Since for each case the relative variation of the scattered field amplitude is of interest, the maximum value of the amplitude has been taken to be equal to 1.00. The scattering patterns show that for the cases when the radius of the sphere is comparable to λ the amplitude gradually decreases with the scattering angle θ. For $\rho = 6$, the curve rapidly decreases from a maximum at $\theta = 0°$ to a minimum at $\theta \simeq 35°$ after which the curve becomes oscillating. For $\rho = 2$, the amplitude falls from a maximum at $\theta = 0°$ almost exponentially till $\theta = 135°$ when there is a tendency to rise rather slowly. The curve for $\rho \to 0$ shows that the scattered amplitude gradually increases with θ. Thus, the sphere with $\rho = 2$ is found to behave, of the three cases considered, in a way nearest to that of atoms as far as the scattering curve is concerned. Fig. 3 shows the variations of amplitude of

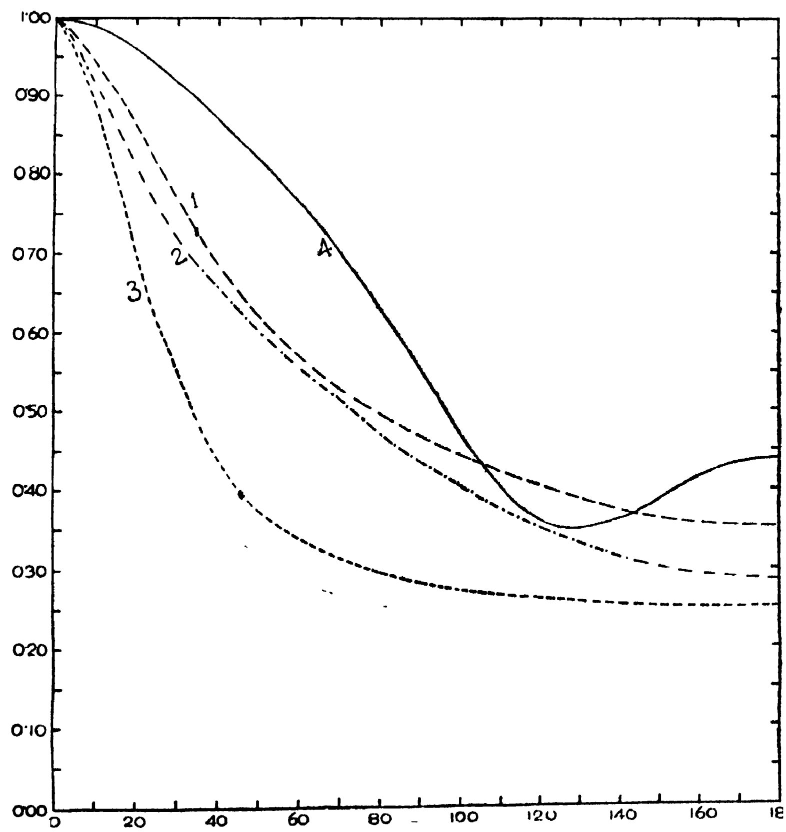

Fig. 3. Variation of the amplitude of X-rays scattered by atoms of copper, aluminium and carbon. Curve 1–copper, Curve 2–aluminium, Curve 3–carbon, Curve 4–scattering pattern of conducting sphere for $\rho = 2.0$.

X-rays scattered by atoms of copper, aluminium and carbon (James and Brinedly, 1931) and for e.m. waves for a conducting sphere with $\rho = 2$. It is observed that the nature of all these curves agree to a large extent. Prehaps better agreement can be achieved with values of ρ which are near to but not exactly equal to 2 or perhaps spheres with different dielectric constants will give better agreement. These cases have not been investigated by us as yet. However, we may safely conclude that with conducting spheres, ρ must have a value very nearly equal to 2 so that the atoms are adequately simulated as far as scattering behaviour is concerned.

REFERENCES

Allen, R. A., 1955, *Am. J. Phys.*, **23**, 297

Blumer, H., 1925, *Z. Physik*, **32**, 119

Blumer, H., 1926a, *Z. Physik*, **38**, 304

Blumer, H., 1926b, *Z. Physik*, **38**, 920

Blumer, H., 1926c, *Z. Physik*, **39**, 195

Jahnke, E. and Emde, F., 1943, Tables of Functions, Dover Publications, New York.

James, R. W., and Brindley, G. W., 1931, *Phil. Mag.*, **12**, 81.

Mie, G., 1908, *Ann. Physik.*, **25**, 377.

Mitra, G. B. and Sanyal, G. S., 1960, *Ind. J. Phys.*, **34**, 103.

Morse, P. M. and Feshback, H., 1953, Methods of Theoretical Physics, Mc-Graw Hill, 1882.

Stratton, J. A., 1941, Electromagnetic Theory, Mc-Graw Hill, 564.

Watson, G. H., 1922, A Treatise on the Theory of Bessel Functions, Cambridge University Press.